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Division of Environmental Chemistry
– Molecular Materials Chemistry –

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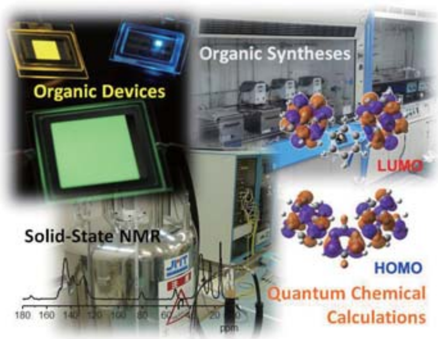
Scope of Research

Our research target is to develop high-performance organic electroluminescence devices, organic solar cells, and polymer materials. For the purpose, we have carried out syntheses, device fabrications, precise structure characterizations, and quantum chemical calculations for high functional organic materials. Along with exploring novel synthetic routes and novel devices, detailed analyses of structures and dynamics are performed mainly by sophisticated solid-state NMR spectroscopy in order to obtain structure-dynamics-property relationships.



KEYWORDS

Solid-State NMR
Amorphous Materials
Organic Solar Cells
Organic Light-Emitting Diodes
Living Radical Polymerization

Selected Publications

Suzuki, F.; Nishiyama, Y.; Kaji, H., Clarification of Isomeric Structures and the Effect of Intermolecular Interactions in Blue-emitting Aluminum Complex Alq_3 Using First-principles ^{27}Al NMR Calculations, *Chemical Physics Letters*, **605-606,** 1-4 (2014).

Uejima, M.; Sato, T.; Detani, M.; Wakamiya, A.; Suzuki, F.; Suzuki, H.; Fukushima, T.; Tanaka, K.; Murata, Y.; Adachi, C.; Kaji, H., A Designed Fluorescent Anthracene Derivative: Theory, Calculation, Synthesis, and Characterization, *Chemical Physics Letters*, **602,** 80-83 (2014).

Lei, L.; Tanishima, M.; Goto, A.; Kaji, H.; Yamaguchi, Y.; Komatsu, H.; Jitsukawa, T.; Miyamoto, M., Systematic Study on Alkyl Iodide Initiators in Living Radical Polymerization with Organic Catalysts, *Macromolecules*, **47,** 6610-6618 (2014).

Lei, L.; Tanishima, M.; Goto, A.; Kaji, H., Living Radical Polymerization via Organic Superbase Catalysis, *Polymers*, **6,** 860-872 (2014).

Clarification of Isomeric Structures and the Effect of Intermolecular Interactions in Blue-emitting Aluminum Complex, Alq_3, Using First-principles ^{27}Al NMR Calculations

Tris(8-hydroxyquinoline) aluminum(III) (Alq_3) has been a widely used light-emitting and electron-transporting material in organic light-emitting diodes. Conventionally, the emission color of Alq_3 has been observed as green; however, recently, blue-emitting Alq_3 have been found. The blue-emitting Alq_3 exhibits photoluminescence quantum yield of ~50%, approximately twofold greater than that of conventional Alq_3. To understand the different luminescent properties, we have performed structure analysis on the blue-emitting Alq_3 using ^{27}Al NMR and first-principles gauge-including projector-augmented wave calculations. From the analysis, we obtained clear evidence that the difference of the luminescent properties originates from the isomeric state of Alq_3 molecules.

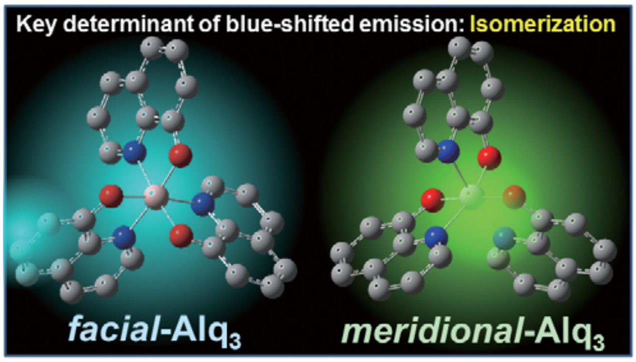


Figure 1. Emission color of Alq_3 is determined by the isomeric state.

Living Radical Polymerization via Organic Superbase Catalysis

Organic superbases reacted with alkyl iodides (R–I) to reversibly generate the corresponding alkyl radicals ($R^{\bullet}$). Via this reaction, organic superbases were utilized as new and highly efficient organic catalysts in living radical polymerization. The superbase catalysts included guanidines, aminophosphines and phosphazenes. Low-polydispersity polymers (M_w/M_n = 1.1–1.4) were obtained up to high conversions (e.g., 80%) in reasonably short times (3–12 h) at mild temperatures (60–80 °C) for methyl methacrylate, styrene and several functional methacrylates. The high polymerization rate and good monomer versatility are attractive features of these superbase catalysts.

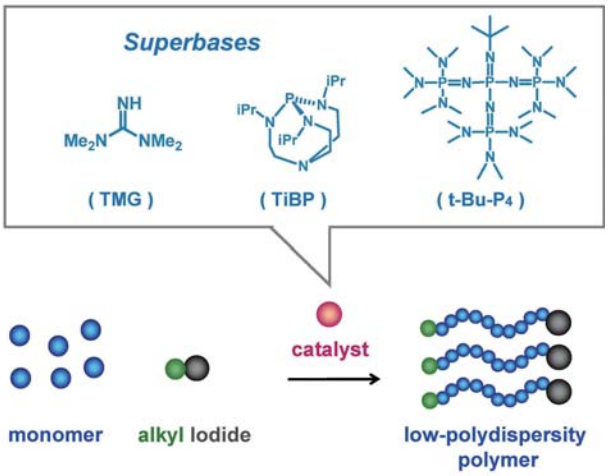


Figure 2. Living Radical Polymerization via Organic Superbase Catalysis.